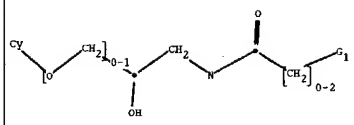
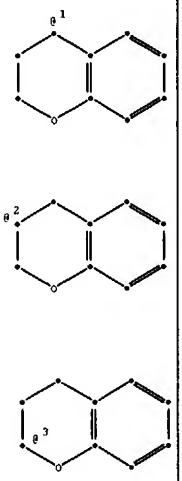
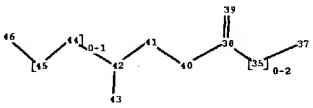
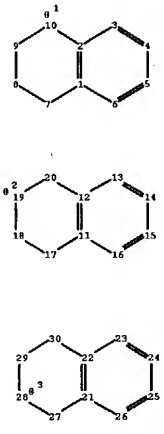
C:\Program Files\Stnexp\Queries\10667286.









chain nodes :
35 37 38 39 40 41 42 43 44 45 46
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
22 23 24 25 26 27 28 29 30
chain bonds :
35-37 35-38 38-39 38-40 40-41 41-42 42-43 42-44 44-45 45-46
ring bonds :
1-2 1-6 1-7 2-3 2-10 3-4 4-5 5-6 7-8 8-9 9-10 11-12 11-16 11-17
12-13 12-20 13-14 14-15 15-16 17-18 18-19 19-20 21-22 21-26 21-27
22-23 22-30 23-24 24-25 25-26 27-28 28-29 29-30
exact/norm bonds :
35-37 38-39 38-40 42-43 45-46
exact bonds :
1-7 2-10 7-8 8-9 9-10 11-17 12-20 17-18 18-19 19-20 21-27 22-30
27-28 28-29 29-30 35-38 40-41 41-42 42-44 44-45
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
21-22 21-26 22-23 23-24 24-25 25-26
isolated ring systems :
containing 1 : 11 : 21 :

G1:[*1],[*2],[*3]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 35:CLASS 37:CLASS 38:CLASS
39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS
46:Atom

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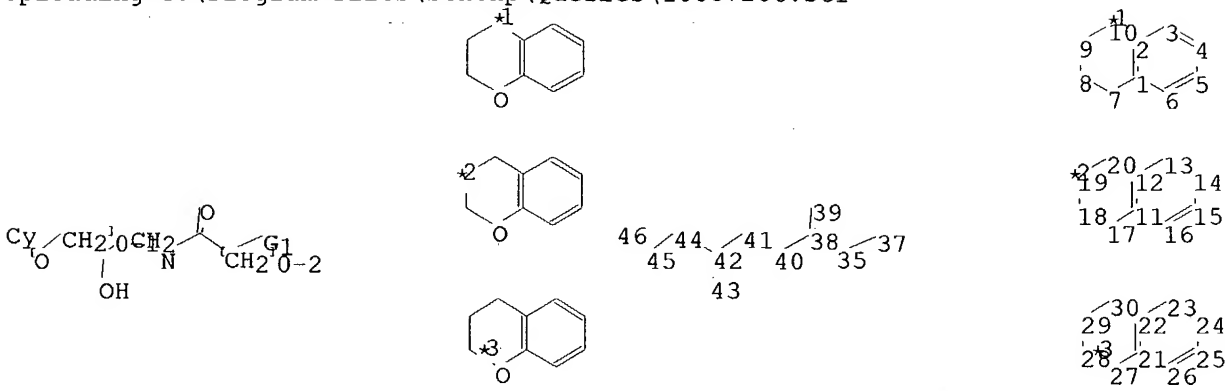
Uploading C:\Program Files\Stnexp\Queries\10667286.str



chain nodes :
35 37 38 39 40 41 42 43 44 45 46
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30
chain bonds :
35-37 35-38 38-39 38-40 40-41 41-42 42-43 42-44 44-45 45-46
ring bonds :
1-2 1-6 1-7 2-3 2-10 3-4 4-5 5-6 7-8 8-9 9-10 11-12 11-16 11-17 12-13 12-20 13-14 14-15 15-16 17-18 18-19 19-20 21-22 21-26 21-27 22-23 22-30 23-24 24-25 25-26 27-28 28-29 29-30
exact/norm bonds :
35-37 38-39 38-40 42-43 45-46
exact bonds :
1-7 2-10 7-8 8-9 9-10 11-17 12-20 17-18 18-19 19-20 21-27 22-30 27-28 28-29 29-30 35-38 40-41 41-42 42-44 44-45
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 21-22 21-26 22-23 23-24 24-25 25-26
isolated ring systems :
containing 1 : 11 : 21 :

G1:[*1],[*2],[*3]

```
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom
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29:Atom  30:Atom  35:CLASS  37:CLASS  38:CLASS  39:CLASS  40:CLASS  41:CLASS
42:CLASS  43:CLASS  44:CLASS  45:CLASS  46:Atom



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 17:29:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    390 TO ITERATE

100.0% PROCESSED     390 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         6616 TO     8984
PROJECTED ANSWERS:               2 TO      124

L2            2 SEA SSS SAM L1

=> => s l1 sss ful
FULL SEARCH INITIATED 17:31:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   7819 TO ITERATE

100.0% PROCESSED    7819 ITERATIONS                                10 ANSWERS
SEARCH TIME: 00.00.01

L3           10 SEA SSS FUL L1

=> => s l3
L4           4 L3

=> d l4 1-4 bib,ab,hitstr
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L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:832787 CAPLUS
DN 137:337786
TI Preparation of chiral alkylaminochroman derivatives as β3-adrenoreceptor agonists
IN O'Connor, Stephen J.; Ladouceur, Gaetan H.; Bullock, William H.; Campbell, Ann-Marie; Dai, Miao; Dally, Robert; Dumas, Jacques; Hatoum-Mokdad, Holia N.; Khire, Uday; Lee, Wendy; Liu, Qingjie; Lowe, Derek B.; Magnuson, Steven R.; Qi, Ning; Shelekhin, Tatiana E.; Shen, Quanrong; Smith, Roger A.; Wang, Ming
PA Bayer Corporation, USA
SO PCT Int. Appl., 193 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002085891	A1	20021031	WO 2002-US12940	20020422
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003078260	A1	20030424	US 2002-131448	20020422
	US 6660752	B2	20031209		
	EP 1389202	A1	20040218	EP 2002-723958	20020422
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2004072828	A1	20040415	US 2003-666903	20030917
PRAI	US 2001-285719P	P	20010423		
	US 2001-324518P	P	20010926		
	US 2002-131448	A1	20020422		
	WO 2002-US12940	W	20020422		

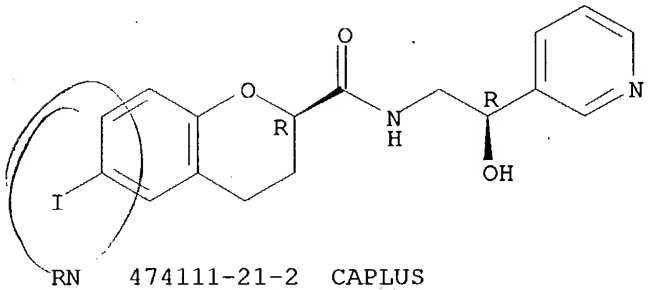
OS MARPAT 137:337786
AB This invention relates to novel 2,6-substituted chroman derivs. which are useful in the treatment of β3-adrenoreceptor mediated conditions. Title compds. I [wherein R = independently OH, :O, halo, CN, NO2, (halo)alkyl, CF3, NR1R1, SR1, OR1, SO2R2, OCOR2, NR1COR2, COR2, NR1SO2R2, or (un)substituted Ph or heterocyclyl; R1 = independently H, (CH2)mO(CH2)mR5, or (un)substituted (cyclo)alkyl, Ph, or naphthyl; or NR1R1 = heterocyclyl; R2 = independently R1, OR1, NR1R1, or (un)substituted NHSO0-2-Ph, NHSO0-2-naphthyl, NHSO0-2-alkyl, or heterocyclyl; R3 = H, alkyl, or COR3; R4 = H, alkyl(phenyl), or alkylpyridyl; R5 = H or CO2H; R6 = H or (un)substituted alkyl or alkyl-SO0-2-alkyl; Ar = Ph or (fused) hetero(aryl); Y = halo, NO2, R6, SR1, SO0-2C6H4CO2R1, (CONR4CR4R4)pCO2R1, or (un)substituted Ph or heterocyclyl; m = 1-3; n = 0-5; p = 1 or 2; and pharmaceutically acceptable salts and esters thereof] were prepared as β3-adrenoceptor agonists. For example, coupling of (2R)-6-iodo-3,4-dihydro-2H-chromene-2-carboxylic acid and (1R)-2-amino-1-(3-pyridinyl)ethanol•2HCl with 1-hydroxybenzotriazole, 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide•HCl, and TEA in CH2Cl2 gave the amide (74%). Reduction using borane-dimethylsulfide complex in THF afforded the

chromanmethaneamine II (84%). Over one hundred compds. of the invention demonstrated β3-adrenergic receptor agonist activity with EC50 values ≤ 1μM. I are useful in the treatment of β3-adrenergic receptor mediated conditions, including obesity, diabetes, gastrointestinal disorders, cardiovascular disorders, and urinary disorders (no data).

IT **474111-20-1P**, (2R)-N-[(2R)-2-Hydroxy-2-(3-pyridinyl)ethyl]-6-iodo-3,4-dihydro-2H-chromene-2-carboxamide **474111-21-2P**, (2S)-N-[(2R)-2-Hydroxy-2-(3-pyridinyl)ethyl]-6-iodo-3,4-dihydro-2H-chromene-2-carboxamide **474112-71-5P**, (2R)-N-[(2R)-2-Hydroxy-2-(3-pyridinyl)ethyl]-6-nitro-3,4-dihydro-2H-chromene-2-carboxamide **474114-45-9P**, (2R)-N-[(2R)-2-[6-(2,5-Dimethyl-1H-pyrrol-1-yl)-3-pyridinyl]-2-hydroxyethyl]-6-iodo-3,4-dihydro-2H-chromene-2-carboxamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(β3-adrenoreceptor agonist; preparation of chiral alkylaminochroman derivs. as β3-adrenoreceptor agonists)

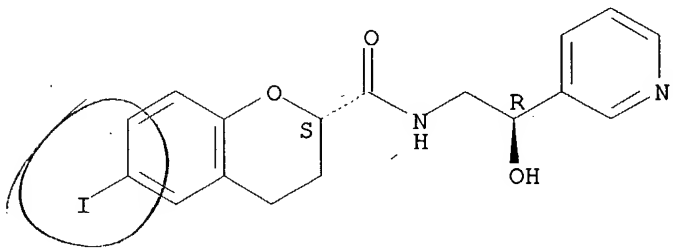
RN 474111-20-1 CAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 3,4-dihydro-N-[(2R)-2-hydroxy-2-(3-pyridinyl)ethyl]-6-iodo-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



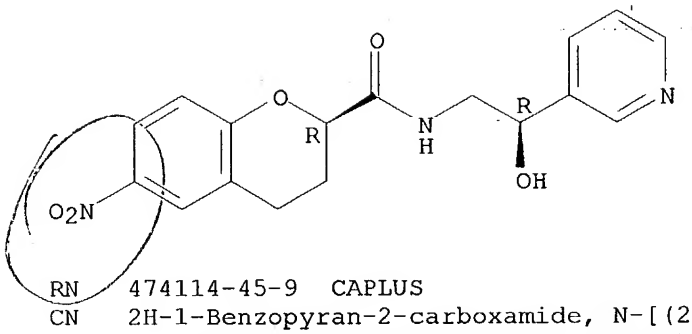
RN 474111-21-2 CAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 3,4-dihydro-N-[(2R)-2-hydroxy-2-(3-pyridinyl)ethyl]-6-iodo-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



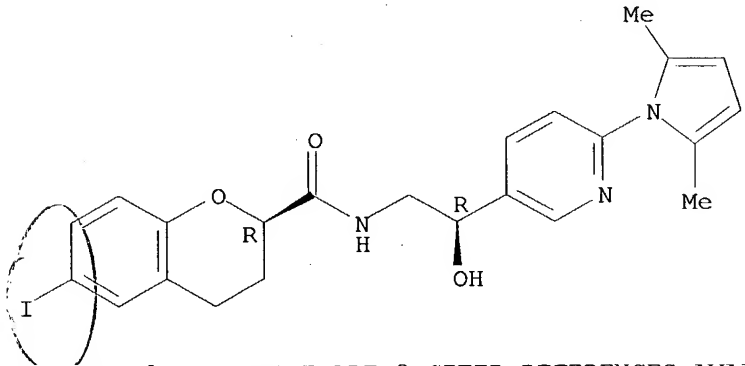
RN 474112-71-5 CAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 3,4-dihydro-N-[(2R)-2-hydroxy-2-(3-pyridinyl)ethyl]-6-nitro-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 474114-45-9 CAPLUS
CN 2H-1-Benzopyran-2-carboxamide, N-[(2R)-2-[6-(2,5-dimethyl-1H-pyrrol-1-yl)-3-pyridinyl]-2-hydroxyethyl]-3,4-dihydro-6-iodo-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:465994 CAPLUS
DN 137:33326
TI Preparation of chiral alkylaminochroman derivatives as β3 adrenoreceptor agonists
IN Ladouceur, Gaetan H.; Bullock, William H.; Magnuson, Steven R.; O'Connor, Stephen J.; Smith, Roger A.; Shen, Quanrong; Liu, Quingjie; Su, Ning; Velthuisen, Emil J.; Campbell, Ann-Marie; Ehrlich, Paul P.
PA Bayer Corporation, USA
SO PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002048134	A2	20020620	WO 2001-US46623	20011207
	WO 2002048134	A3	20030206		
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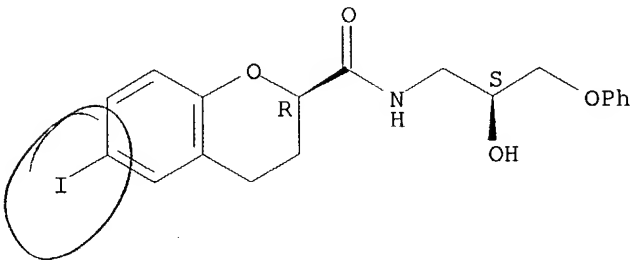
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002028816	A5	20020624	AU 2002-28816	20011207
	US 2003078258	A1	20030424	US 2001-8928	20011207
	US 6699860	B2	20040302		
	EP 1343778	A2	20030917	EP 2001-989934	20011207
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004524286	T2	20040812	JP 2002-549665	20011207
PRAI	US 2000-254735P	P	20001211		
	WO 2001-US46623	W	20011207		

OS MARPAT 137:33326
AB Title compds. [I; Ar = C6H5, heterocycle, benzoheterocycle; Y = halo, OR1, COOR1, CH2CH2COOH, 4-C6H4COOH, 4-C6H4COOCH3, 3-C6H4COOH, 2-naphthyl-6-carboxylic acid, etc.; m = 0, 1, 2, 3, 4, 5; n = 1, 2, 3; X = O, S, S:O, SO2; R = OH, halo, CN, NO2, CF3; R1 = H, (CH2)nO(CH2)nCOOH, (CH2)nO(CH2)nH; R2 = R1, OR1, NR1R1, alkoxy, halo, NO2; R3 = H, alkyl, C6H5CH2, COR2] are prepared as β3 adrenergic receptor agonists. Title compds. I are useful in a pharmaceutical composition for the treatment of diabetes, impaired fasting glucose, impaired glucose tolerance, obesity, hypertriglyceridemia, hypercholesterolemia, hypercholesterolemia, lowering high-d. lipoprotein levels, atherosclerosis, cardiovascular diseases and related diseases, gastrointestinal disorders, neuro genetic inflammation, ocular hypertension, glaucoma, urol. disorders, benign prostatic hyperplasia, and, incontinence. Thus, the title compound II was prepared from (2R)-t-iodo-3,4-dihydro-2H-chroman-2-carboxylic acid, Me 4-iodobenzoate, and (2S)-1-amino-3-phenoxy-2-propanol via reduction and condensation. The title compound II was tested for β3 agonistic activity with EC50 ≤ 1μM.
IT **437764-11-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral aminoalkylchroman derivs. as β3 adrenoreceptor

agonists)
RN 437764-11-9 CAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 3,4-dihydro-N-[(2S)-2-hydroxy-3-phenoxypropyl]-6-iodo-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:421677 CAPLUS
DN 131:73558
TI Preparation of chromansulfonamides as β-3 adrenoreceptor agonists
IN Ladouceur, Gaetan H.; Connell, Richard D.; Baryza, Jeremy; Campbell, Ann-Marie; Lease, Timothy G.; Cook, James H.
PA Bayer Corporation, USA
SO PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DT Patent
LA English

Appl. PCT

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9932475	A1	19990701	WO 1998-US24627	19981117
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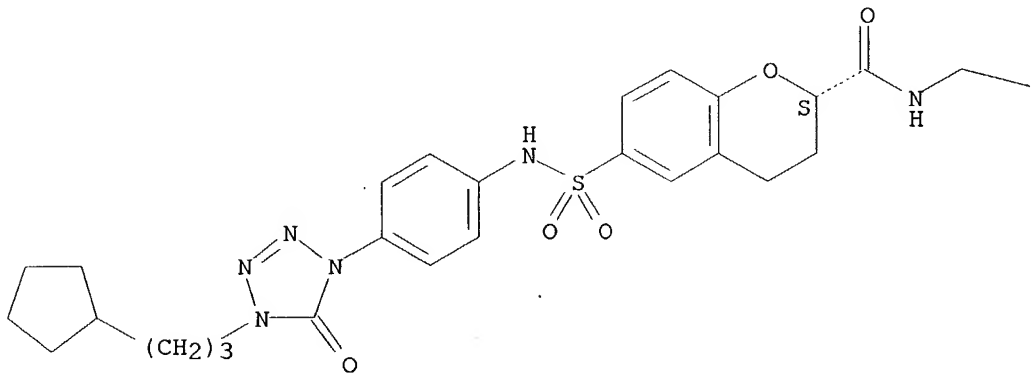
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	ZA 9810489	A	19990520	ZA 1998-10489	19981117
	CA 2314925	AA	19990701	CA 1998-2314925	19981117
	AU 9914183	A1	19990712	AU 1999-14183	19981117
	AU 751015	B2	20020808		
	EP 1054881	A1	20001129	EP 1998-958070	19981117
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2001526281	T2	20011218	JP 2000-525412	19981117
	TW 502032	B	20020911	TW 1998-87118968	19981117
	US 6051586	A	20000418	US 1998-199014	19981123
	US 2003073839	A1	20030417	US 2000-520201	20000307
	US 2004072843	A1	20040415	US 2003-667286	20030919 ← Appl.
PRAI	US 1997-994585	A	19971219		
	US 1997-122061P	P	19971219		
	WO 1998-US24627	W	19981117		
	US 1998-199014	A3	19981123		
	US 2000-520201	B1	20000307		

OS MARPAT 131:73558
AB Title compds. [I; R = H, OH, O, halo, haloalkyl, alkyl, cyano, NO2, N(R1)2, SR1, OR1, SO2R2, CO2R2, COR2, NR1SO2R2, NR1COR2; R1 = H, (substituted) alkyl, cycloalkyl, Ph, naphthyl; R2 = R1, N(R1)2; R3 = H, alkyl, RAr1CH(OH)CH2; Ar1 = Ar1OCH2, Ph, (fused) heterocyclyl; m = 1-3; n = 0-4; X = piperazinylsulfonyl, NR3SO2; Ar2 = (substituted) (fused) Ph, heterocyclyl; Y = OY, NR1, NR1CO, (oxo-substituted) cycloalkyl, heterocyclyl; p = 0, 1; R4 = H, R1, R2, oxo, (substituted) heteroalkyl, alkyl, haloalkyl], were prepared for treatment of diabetes and obesity (no data). Thus, (R)-(pyrid-3-yl)oxirane (preparation given) and 2-aminomethylchroman-6-sulfonic acid [4-[4-(3-cyclopentylpropyl)-5-oxo-4,5-dihydrotetrazol-1-yl]phenyl]amide (preparation given) were refluxed in EtOH/H2O to give 11% title compound (II).
IT **228710-21-2P 228710-31-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of chromansulfonamides as β-3 adrenoreceptor agonists)

RN 228710-21-2 CAPLUS
CN 2H-1-Benzopyran-2-carboxamide, 6-[[[4-[4-(3-cyclopentylpropyl)-4,5-dihydro-5-oxo-1H-tetrazol-1-yl]phenyl]amino]sulfonyl]-N-[(2R)-2-[6-(2,5-dimethyl-1H-pyrrol-1-yl)-3-pyridinyl]-2-hydroxyethyl]-3,4-dihydro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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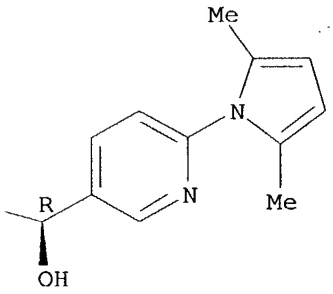

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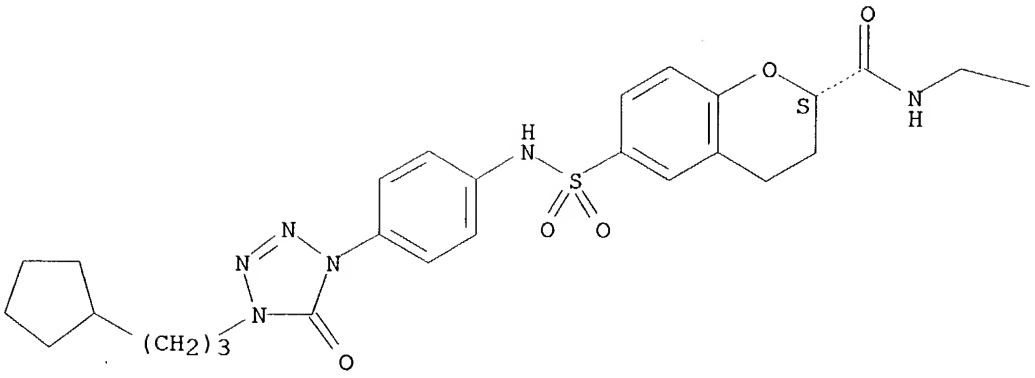
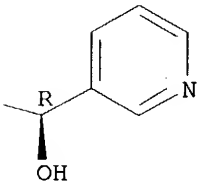
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

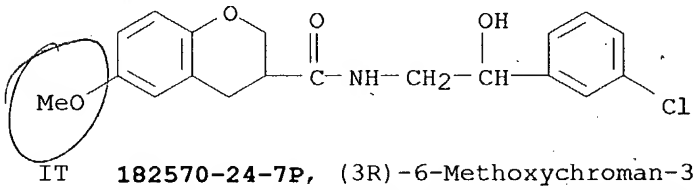


RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:646308 CAPLUS
DN 125:300822
TI Preparation of N-chromanyl and N-chromanylmethyl 2-amino-1-phenylethanol compounds as adrenergic β3-receptor stimulants
IN Tsucha, Susumu; Fukuzaki, Atsushi; Takenawa, Noriko; Ozaka, Kazuya
PA Tokyo Tanabe Co, Japan
SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

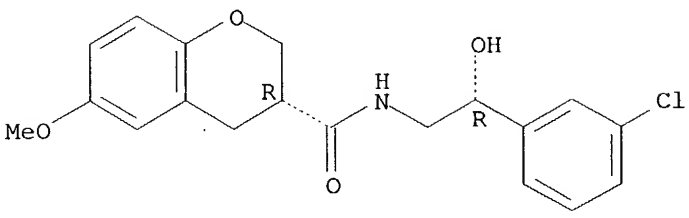
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 08198866	A2	19960806	JP 1995-6912	19950120
PRAI JP 1995-6912		19950120		

OS MARPAT 125:300822
AB The title compds. (I; X = H, halo; n = 0-1; Y = H, OH, lower alkoxy, carboxymethoxy, lower alkoxycarbonylmethoxy)and their pharmacol. acceptable salts are prepared I show intestinal motility inhibition and antidiarrhea activity and are useful for the treatment of gastrointestinal diseases accompanied by unusual tension of smooth muscle. Thus, 6-methoxychroman-3-carboxylic acid (2R)-[2-(3-chlorophenyl)-2-hydroxyethyl]amide (preparation given) was reduced by BH3.Et2S in THF to give (1R) I (X = 3-Cl, n = 0, Y = 6'-OMe), which inhibited 60% diarrhea at 1 mg/kg p.o. in rats.
IT **182570-13-4P**, 6-Methoxychroman-3-carboxylic acid [2-(3-chlorophenyl)-2-hydroxyethyl]amide
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-amino-1-phenylethanol compds. as adrenergic β3-receptor stimulators for treatment of gastrointestinal diseases)
RN 182570-13-4 CAPLUS
CN 2H-1-Benzopyran-3-carboxamide, N-[2-(3-chlorophenyl)-2-hydroxyethyl]-3,4-dihydro-6-methoxy- (9CI) (CA INDEX NAME)



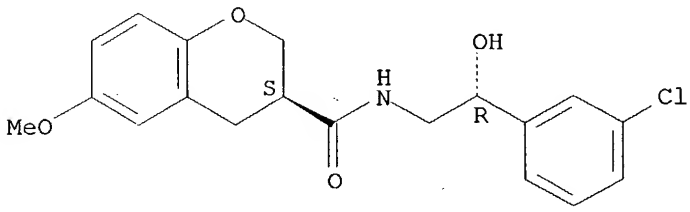
IT **182570-24-7P**, (3R)-6-Methoxychroman-3-carboxylic acid 2R-[2-(3-chlorophenyl)-2-hydroxyethyl]amide **182821-95-0P**, (3S)-6-Methoxychroman-3-carboxylic acid (2R)-[2-(3-chlorophenyl)-2-hydroxyethyl]amide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-amino-1-phenylethanol compds. as adrenergic β3-receptor stimulators for treatment of gastrointestinal diseases)
RN 182570-24-7 CAPLUS
CN 2H-1-Benzopyran-3-carboxamide, N-[2-(3-chlorophenyl)-2-hydroxyethyl]-3,4-dihydro-6-methoxy-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 182821-95-0 CAPLUS
CN 2H-1-Benzopyran-3-carboxamide, N-[2-(3-chlorophenyl)-2-hydroxyethyl]-3,4-dihydro-6-methoxy-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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